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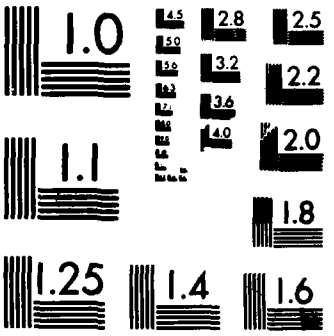

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This report describes research undertaken at the Research Institute of Colorado on two computational mathematics topics: algebraic multigrid (AMG), and the fast adaptive composite grid method (FAC).

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ALGEBRAIC MULTIGRID AND THE FAST ADAPTIVE COMPOSITE GRID METHOD IN LARGE SCALE COMPUTATION

Dr. Stephen F. McCormick

Research Institute of Colorado
Drake Creekside Two, Suite 200
2629 Redwing Road
Ft. Collins, Colorado 80526

for the

Air Force Office of Scientific Research

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Final Report

Algebraic Multigrid and the Fast Adaptive Composite Grid Method in Large Scale Computation

Progress of this project is categorized into the two areas described below.

I. AMG. The first area is devoted to study of algebraic multigrid (AMG) (cf. (1)-(8)).

Conventional or geometric multigrid algorithms depend on knowledge of the underlying geometry for a given problem (e.g., a partial differential equation). This knowledge is used to predetermine coarser grids and the attendant operators and intergrid transfers. Although very efficient solvers can be developed in this way, the dissemination and use of geometric multigrid have been impeded by the need to tailor the algorithm to each application. A fairly general "black box" solver based on multigrid principles would be useful in overcoming these difficulties. In fact, AMG is such a scheme that has many advantages over other solvers (cf. (7)) for treating many complex and irregular problems (cf. the introductions to (1) and (2)).

For certain classes of matrices (e.g., symmetric positive-type), the project has established AMG as an effect "black box" solver: the research has shown (2) that point Gauss-Seidel for such matrices achieves (algebraic) smoothness in the sense that the errors after just a few sweeps are "locally constant"; that is, variables that are strongly coupled via large off-diagonal matrix entries must have similar errors. The coarsening process may therefore use a Ritz-type variational formulation in an attempt to approximate such errors; that is, it is enough to determine an interpolation process that ensures that such errors are approximately in the range of interpolation. Such an approximation property must be achieved while maintaining low complexity of the resulting coarse-level problems; this can generally be accomplished by an "operator" interpolation scheme that uses the matrix to determine the interpolation coefficients. More critically, the coarse grid variables themselves are chosen automatically in this scheme so that they properly represent the "strength" of the fine grid equations. Loosely speaking, each fine grid

variable that is not rexerved for the coarse grid must have only strong couplings to variables that either are themselves reserved for the coarse grid or are strongly coupled to variables that are. The means for implementing this "coarsening" process are quite intricate, but the objectives that guide it are fairly straightforward. Moreover, sharp convergence rates were proved in this and in more general cases, including block positive-type matrices such as those that arise from discretizing Stokes equations (cf. (2)).

The main difficulty in applying AMG to new classes of matrices is one of determining the sense of smoothness (of relaxed errors) for these classes. This sense is used as a basis for the coarsening process to determine strong cou;lings and for interpolation to determine how to "collapse" the operator (i.e., how to ignore couplings between strictly fine grid points so that a fine grid variable is determined purely by coarse grid ones). Automatic ways for computationally detecting the sense of smoothness that use preliminary relaxation sweeps were one of the central focuses of the project.

The project studied AMG applied to a wide variety of essentially positive-type problems, including anisotropic and ill-behaved diffusion equations as well certain nonsymmetric problems, especially convection dominated diffusion equations (5), (6), and some purely algebraic problems that arise in geodesy (1). And it has just recently been established for many problems in structural mechanics and fluid flows (14). Yet there is a need to continue much of the present efforts to extend AMG to a broader class of problems, applications and machines, and to develop software. There are currently many ideas in each of these directions -- they are in fact quite abundant -- and the study devoted effort to most of them. The project was impelled by important application areas where AMG seems most needed. This included, for example, finite-element and boundary-element discretizations in structural analysis and aerodynamics (the main topics of study), moving grid applications in reaction-diffusion modeling, and many adaptive discretizations applications.

II. FAC. The second project area was the study of FAC in the context of multiprocessor computer systems. FAC is developed for elliptic equations in (9) - (11), which include various descriptions of basic and more sophisticated FAC schemes. Its application to advanced computers is documented in (12) - (13).

There is a clear need for local resolution in many physical phenomena. For example, when special local features of the forcing function, boundary, or coefficients of an elliptic boundary value problem dictate discretization error characteristics that are substantially different than the global features of the problem, it is important that the discretization account for this locally. The presence of, say, a point source should not demand a fine mesh throughout the region. Yet this objective of adapting to local phenomena is often in conflict with the process designed to solve the discrete system. Many linear solvers degrade significantly in the presence of different discretization scales and discrete "interfaces". In fact, even the discretization process itself can be adversely affected by this objective: for finite differences, it is problematic to develop sound difference formulae and data structures to handle nonuniform grids; for finite elements, this objective is reflected in the substantial overhead costs in automating the discretization.

It is, therefore, important to develop mesh refinement techniques that are both efficient as well as systematic. Many existing mesh refinement methods (especially those that are adaptive) are systematic but troubled by slow or expensive solvers; many others (especially MLAT-type schemes (16, (17)) are efficient but can be somewhat ad hoc. FAC attempts to draw from the best of both approaches.

The need for high local resolution is demanding not only better numerical methods, but more advanced computing systems as well. Present and future computational requirements are beyond the reach of expected computer technological advancements and must therefore be addressed by advanced architectures. This is especially true for problems that require high local resolution because one of the basic tenets here is that this is often well beyond present machine capabilities. Parallel architectures appear to be very natural responses to such computational demands, especially in conjunction with FAC since it partitions the local computations into separate independent processes. The combination of FAC and advanced parallel systems can provide a very effective tool for solving a wide variety of large scale computational models.

The recent progress of the project on linear FAC is documented in detail in (12) attached. To summarize, the results include a fairly complete theoretical treatment of convergence and its rates for elliptic problems; a theoretical treatment for the case where the coarse grid operator and/or the fine grid operator are replaced by approximate solvers; a discussion of how to

construct acceptable composite grid operators; numerical results for two types of elliptic problems, a discussion of other topics such as removal of singularities and multilevel FAC; results on the application of FAC to the HEP; complexity analysis of FAC for multiprocessor systems (the first of its kind); and a theoretical and practical development of RQMG, a new and efficient FAC method for eigenvalue problems.

RQMG (13) is a fully variational multigrid-like method for solving differential eigenvalue problems. It has been successfully applied to model problems and to the difficult single group neutron diffusion problem at LANL in cooperation with Joel Dendy. Initial efforts were made to implement an efficient FAC version of RQMG (which has been done on model problems only, but with great success) and to extend these codes to multigroup problems.

Stephen F. McCormick, Ph.D.
Principal Investigator

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